Artificial Intelligence for Drug Discovery: Are We There Yet?

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Abstract

Drug discovery is adapting to novel technologies such as data science, informatics, and artificial intelligence (AI) to accelerate effective treatment development while reducing costs and animal experiments. AI is transforming drug discovery, as indicated by increasing interest from investors, industrial and academic scientists, and legislators. Successful drug discovery requires optimizing properties related to pharmacodynamics, pharmacokinetics, and clinical outcomes. This review discusses the use of AI in the three pillars of drug discovery: diseases, targets, and therapeutic modalities, with a focus on small-molecule drugs. AI technologies, such as generative chemistry, machine learning, and multiproperty optimization, have enabled several compounds to enter clinical trials. The scientific community must carefully vet known information to address the reproducibility crisis. The full potential of AI in drug discovery can only be realized with sufficient ground truth and appropriate human intervention at later pipeline stages. Expected final online publication date for the Annual Review of Pharmacology and Toxicology, Volume 64 is January 2024. Please see http://www.annualreviews.org/page/journal/pubdates for revised estimates.